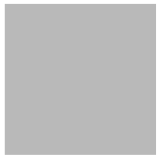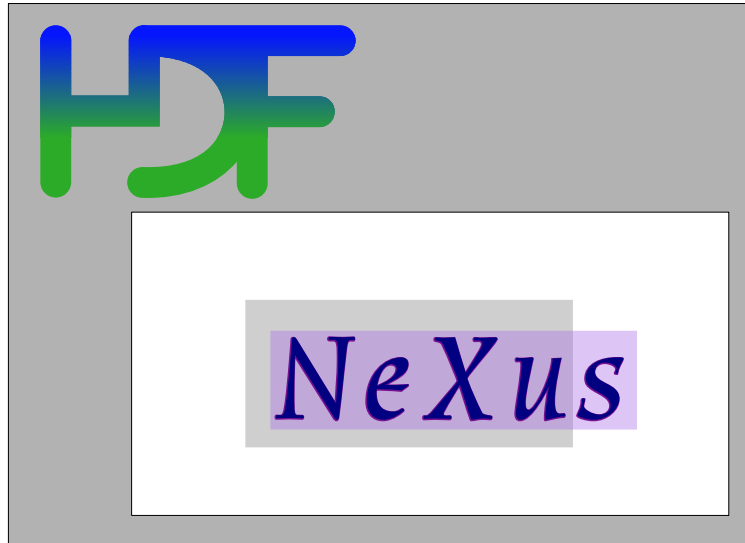WIR SCHAFFEN WISSEN – HEUTE FÜR MORGEN

Benjamin Watts :: PolLux Beamline Scientist :: Paul Scherrer Institut
Chair of NeXus International Advisory Committee

The NeXus Data Format and the NIAC
(NeXus International Advisory Committee)
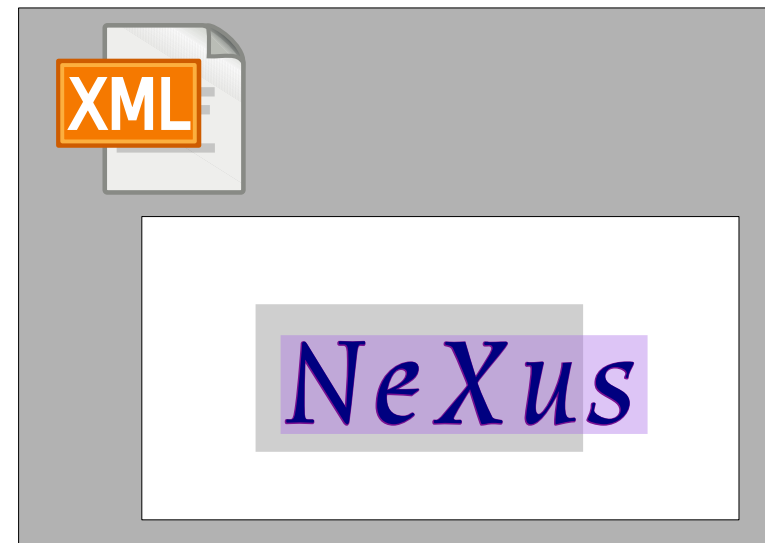
A **file format** describes the encoding of data in binary

A **data format** describes the organisation data within a file

Not NeXus

NeXus

Data storage device ⇒ File system ⇒ File format ⇒ | Data format ⇒ Data hierarchy ⇒ Data types

Excel

NeXus

We currently *recommend* and provide tools for HDF5, but make no *requirement*.
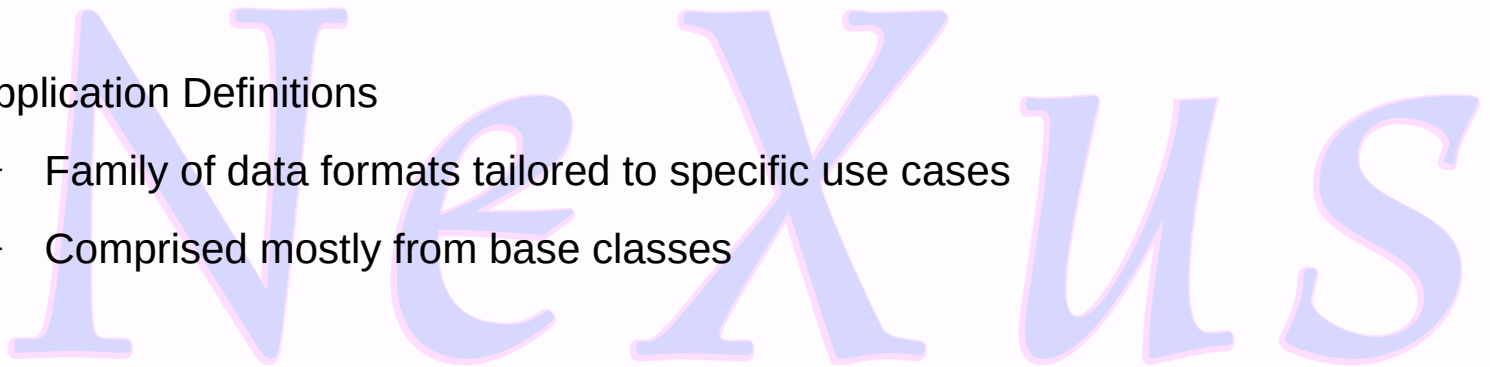We welcome volunteers to extend tools and implement NeXus in other file formats.

Not NeXus   NeXus

Data storage device ⇒ File system ⇒ File format ⇒ Data format ⇒ Data hierarchy ⇒ Data types

- Base Classes

  - Common *building blocks*

  - Set of names with defined spelling and meaning

- Application Definitions

  - Family of data formats tailored to specific use cases

  - Comprised mostly from base classes

- Organisational Framework

  - Formal Processes

    - Proposing and approving additions and changes
    - Democratic representation via the NIAC

  - Community Support

Base Classes

Each NeXus base class represents some object or quantity and provides a set of optional parameters that can describe it.

Each of these parameters (called a **field**) has:

- A **name** (with a specified spelling)

- a **value** (with specified data type)

You can consider the base classes as a set of *recommended* building blocks.

NXaperture

A beamline aperture.

NXattenuator

A device that reduces the intensity of a beam by attenuation.

NXbeam

Properties of the neutron or X-ray beam at a given location.

NXbeam_stop

A device that blocks the beam completely, usually to protect a detector.

NXbending_magnet

A bending magnet

NXcapillary

A capillary lens to focus the X-ray beam.

NXcite

A literature reference

NXcollection

An unvalidated set of terms, such as the description of a beam line.

NXcollimator

A beamline collimator.

NXentry

Top-level group comprising a single measurement.

NXsubentry

An extra level of hierarchy to allow multiple application definitions.

NXdata

NXdata describes the plottable data and related dimension scales.

NXdetector

A detector, detector bank, or multidetector.

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A NeXus application definition defines the set of (required or optional) terms to be used in an instance of that class.

Each application definition is tailored to a specific community.

An application definition is typically constructed from base classes, but can add or adapt fields where needed.

We welcome proposals for new application definitions and for additions* to existing ones.

*we try to avoid changing the meaning of existing fields.

NXarchive

This is a definition for data to be archived by ICAT.

NXarpes

This is an application definition for angular resolved photo electron spectroscopy.

NXcanSAS

Implementation of the canSAS standard to store reduced small-angle scattering data of any dimension.

NXdirecttof

This is a application definition for raw data from a direct geometry TOF spectrometer

NXfluo

This is an application definition for raw data from an X-ray fluorescence experiment

NXmonopd

Monochromatic Neutron and X-Ray Powder diffractometer

NXmx

Functional application definition for macromolecular crystallography

NXsas

Raw, monochromatic 2-D SAS data with an area detector

NXstxm

Application definition for a Scanning Transmission X-ray Microscope.

NXtomo

This is the application definition for x-ray or neutron tomography raw data.

NXtomophase

This is the application definition for x-ray or neutron tomography raw data with phase contrast variation at each point.

NeXus Ideology

We want to remove barriers and reduce burdens for interoperability and sharing of scientific data.

We provide strictness:

- ability to define and validate.

We provide flexibility:

- separate application definitions for different communities.

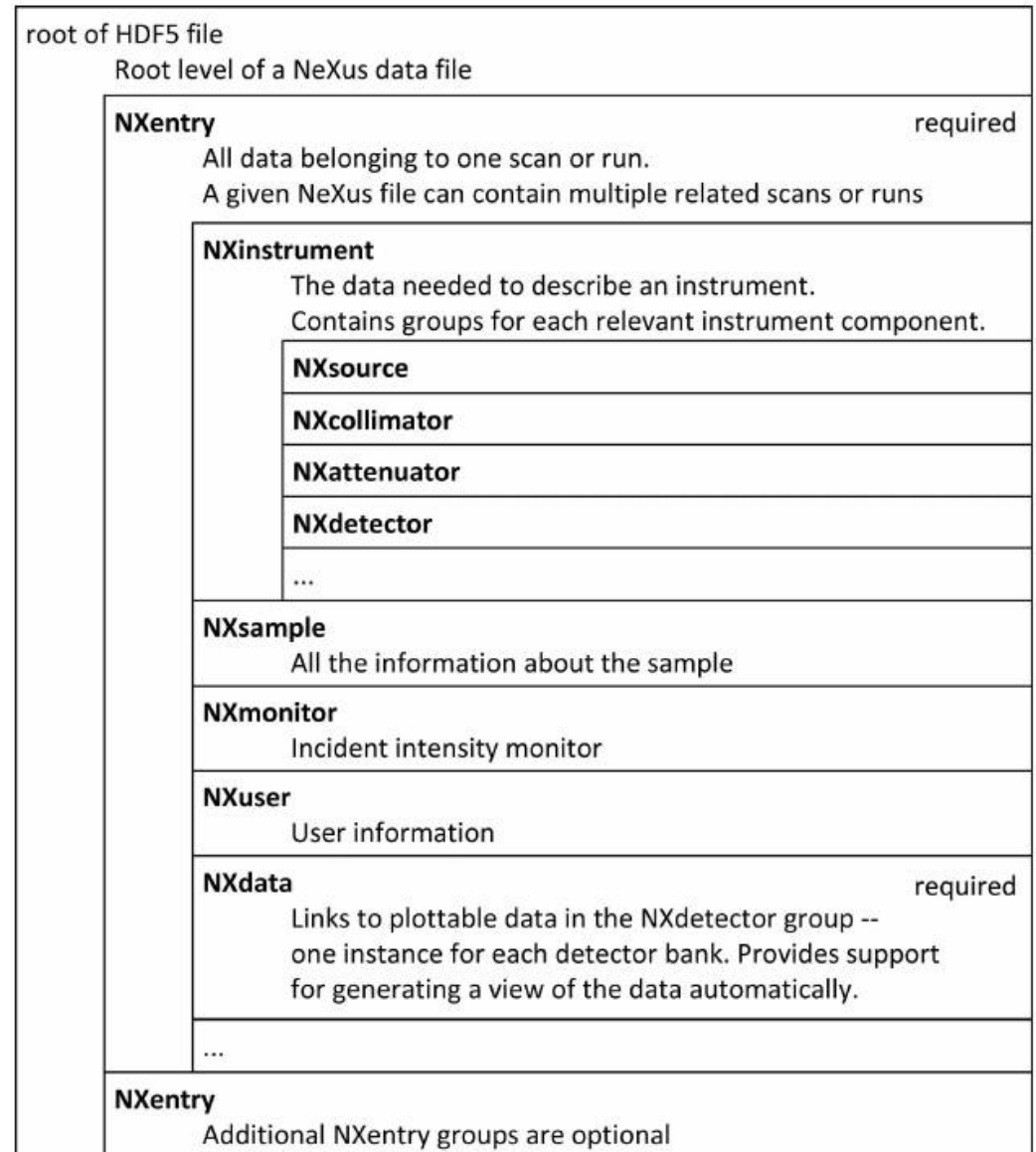- Can always add further data, so long as you respect defined terms.

We recognise the diversity of scientific communities and encourage participation and self-determination.

We cannot achieve a universal standard format in a single step, but commit ourselves to strive for ever-closer cooperation.
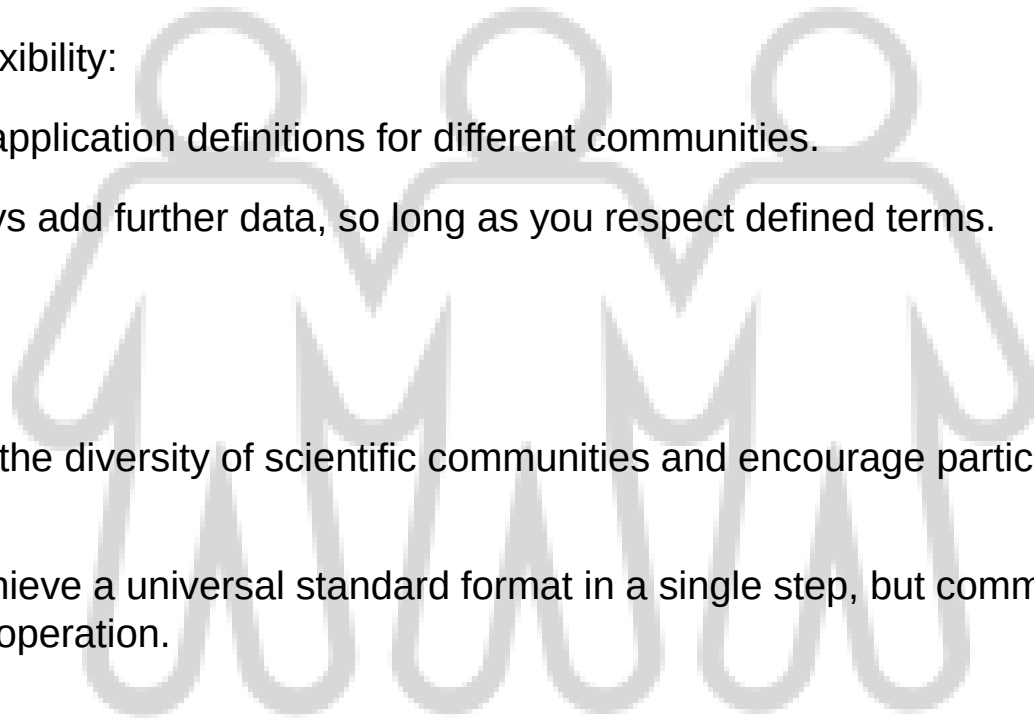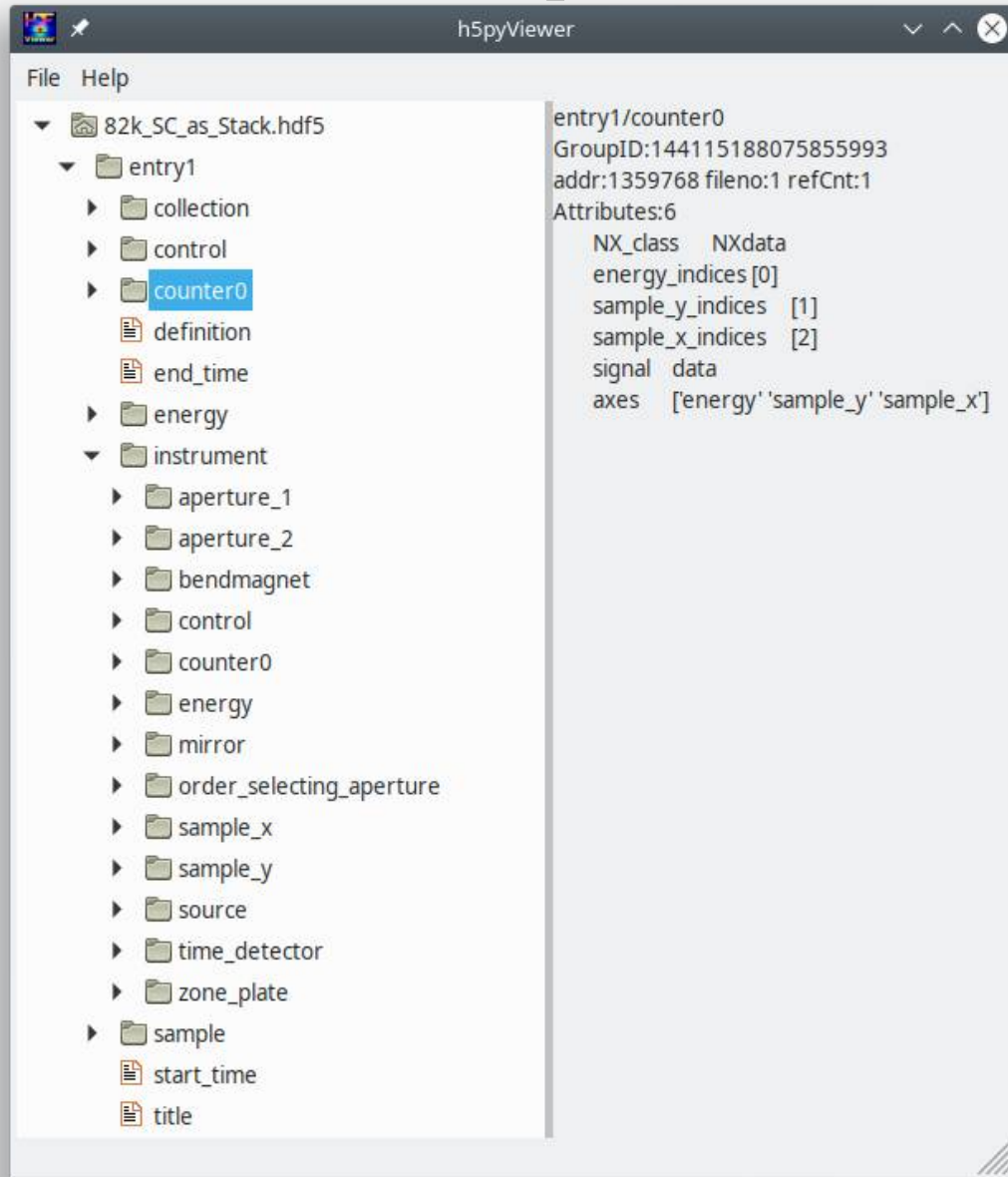
An Example NeXus Structure

- Base classes are implemented as groups and identified via the Nxclass attribute.

- Group names are more flexible to enable human readability.

- An application definition provides required features, but describing the entire experimental apparatus is always encouraged.

root of HDF5 file
Root level of a NeXus data file

NXentry   required
All data belonging to one scan or run.
A given NeXus file can contain multiple related scans or runs

NXinstrument
The data needed to describe an instrument.
Contains groups for each relevant instrument component.

NXsource

NXcollimator

NXattenuator

NXdetector

...

NXsample
All the information about the sample

NXmonitor
Incident intensity monitor

NXuser
User information

NXdata   required
Links to plottable data in the NXdetector group --
one instance for each detector bank. Provides support
for generating a view of the data automatically.

...

NXentry
Additional NXentry groups are optional

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PSI

h5pyViewer

File   Help

- 82k_SC_as_Stack.hdf5
  - entry1
    - collection
    - control
    - counter0
    - definition
    - end_time
    - energy
    - instrument
      - aperture_1
      - aperture_2
      - bendmagnet
      - control
      - counter0
      - energy
      - mirror
      - order_selecting_aperture
      - sample_x
      - sample_y
      - source
      - time_detector
      - zone_plate
    - sample
    - start_time
    - title

entry1/counter0
GroupID:144115188075855993
addr:1359768 fileno:1 refCnt:1
Attributes:6
    NX_class   NXdata
    energy_indices [0]
    sample_y_indices   [1]
    sample_x_indices   [2]
    signal   data
    axes   ['energy' 'sample_y' 'sample_x']

root of HDF5 file
    Root level of a NeXus data file

NXentry
    All data belonging to on
    A given NeXus file can c

NXinstrument
    The data needed
    Contains groups

NXsource

NXcollimator

NXattenuator

NXdetector

...

NXsample
    All the informati

NXmonitor
    Incident intensit

NXuser
    User informatior

NXdata
    Links to plottable
    one instance for
    for generating a

...

NXentry
    Additional NXentry grou

- NeXus International Advisory Committe (NIAC)

    - Members recommended by stakeholder institutions.

    - Mostly from X-ray and neutron facilities.

    - Other types of stakeholders are accepted.

- NIAC activities:

    - Proposed changes and additions discussed and voted on.

    - Full meeting every second year (following NOBUGS conference).

    - Smaller "code camp" meeting in between years.

    - Monthly teleconferences to discuss issues as they arise.

- Mailing lists for general support.

- Github is increasingly used for discussions and proposals.

NeXus International Advisory Committee

Benjamin Watts, Paul Scherrer Institute (Swiss Light Source), Switzerland (Chair)

Freddie Akeroyd, Rutherford Appleton Laboratory (Neutron Source), UK (Executive Secretary)

Stuart Campbell, Brookhaven National Laboratory/NSLS-II, USA (Technical Release Manager)

Peter Chang, Diamond Light Source, UK (Documentation Release Manager)

Herbert Bernstein, CIF (non-facility member)

Aaron Brewster, Lawrence Berkeley Laboratory, USA

Bjørn Clausen, Los Alamos National Laboratory, USA

Stephen Cottrell, Rutherford Appleton Laboratory (Muon Source), UK

Heike Görzig, Helmholtz Zentrum Berlin, Germany

Pete Jemian, Advanced Photon Source, USA

Mark Könnecke, Paul Scherrer Institute (Neutron Source) Switzerland

Raymond Osborn, Argonne National Laboratory, USA (non-facility member)

Wout de Nolf, European Synchrotron Radiation Facility, France

Jiro Suzuki, J-PARC, Japan

Takahiro Matsumoto, Spring8, Japan

Lajos Schrettner, Extreme Light Infrastructure, Czech Republic, Hungary and Romania

Russ Berg, Canadian Light Source, Canada

Sandor Brockhauser, NOMAD Data Center (HU Berlin), Germany

Majid Ounsy, Synchrotron Soleil, France

Chen Zhang, Oak Ridge National Laboratory (SNS/HFIR), USA

Luca Geliso, European XFEL, Germany

Contributing to NeXus

There are many ways to contribute to NeXus:

- Read the manual at https://manual.nexusformat.org/index.html
- Join the mailing list at https://manual.nexusformat.org/mailinglist.html
- Discuss and promote NeXus within your community.
    - Make sure that your community is represented on the NIAC.
- Discuss issues at Github
    - Especially at https://github.com/nexusformat/definitions/issues
    - Provide feedback on (or pull-requests for) the NeXus documentation.
- Ask instrument vendors to write NeXus-compatible files.
- Implement NeXus file writers for your instruments.
    - Propose a new application definition if an appropriate one doesn`t exist yet.
- Implement NeXus file readers for analysis programs.
    - Only corresponding application definitions. It doesn`t make sense to read XPS data into an application for scattering analysis!